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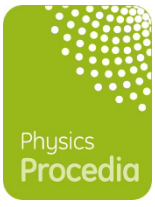

Effect of Lishitz transition on thermal transport properties in Sr_2RuO_4

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Abstract

Inspired by specific features of the spin-triplet superconductor Sr_2RuO_4, we investigate thermal transport properties for a generic chiral p-wave superconductor. One of the bands of Sr_2RuO_4 lies close to a Lifshitz transition which would lead to a change of the Fermi surface topology and influence also topological properties of the chiral superconducting phase characterized by the so-called Chern number. Treating superconductivity based on a two-dimensional tight-binding model for the relevant γ band and a self-consistent Bogoliubov-de Gennes approach, we study thermal transport properties. We focus particularly on the connection between topological properties of the superconducting phase and thermal Hall conductivity. Our results show that low-temperature thermal Hall conductivity can be decomposed into a T-linear contribution and an thermally activated correction, whereby the latter incorporates information about the size of the superconducting gap and the Lifshitz transition.

Keywords: Sr_2RuO_4, chiral p-wave superconductor, topological superconductor

1 Introduction

The transition metal oxide Sr_2RuO_4 has attracted much interest as an unconventional superconductor with presumably spin-triplet Cooper pairing [1, 2, 3]. Experiments such as μSR and polar Kerr effect reveal that the time-reversal symmetry is broken in the superconducting phase [4, 5], advancing the so-called chiral p-wave state as the leading candidate for the pairing symmetry. Using the $\boldsymbol{d}$-vector notation this state is in its most reduced form represented as

$$\boldsymbol{d} \propto \hat{z}(k_x \pm ik_y), \tag{1}$$

with orbital angular momentum $L_z = \pm 1$ of the Cooper pairs along the z axis (two-fold degeneracy), in-plane equal-spin pairing [6] and an excitation gap without symmetry imposed nodes.

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This pairing state is accompanied by topology induced chiral subgap quasiparticle states at the surfaces and domain walls between degenerate phases ($L_z = \pm 1$), which are supposed to carry spontaneous supercurrents [7, 8]. Experiments using scanning Hall probe and scanning SQUID microscopes, however, show only negative results so far [9, 10, 11]. Although supercurrents give rise to spontaneous magnetization of orbital origin, the net field may be suppressed by the spin polarization near the edges generated by the interplay of spin-orbit coupling and interaction effects [12]. The edge currents can also be strongly reduced due to the peculiar band effects [13].

In Sr_2RuO_4 three electronic bands, the so-called α, β and γ bands which are derived from the Ru 4d t_{2g} orbitals, dominate the low-energy physics. While the hole-like α and the electron-like β bands are related and quasi-one-dimensional characters, the γ band is electron like and genuinely two-dimensional. The combined Chern number of the α and β bands vanishes, rendering these bands topologically trivial [12]. In contrast, the γ band yields topologically non-trivial properties. While all bands contribute to the chiral edge currents only the chiral edge state belonging to the γ band is topologically protected [14]. First principles calculations based on density functional theory (DFT) of bulk Sr_2RuO_4 show that the γ band lies near a van Hove point, such that Sr_2RuO_4 is in the vicinity of the Lifshitz transition [15, 16]. It has been suggested that the quasiparticle gap of the superconducting phase is reduced close to the Lifshitz transition making the edge states of the γ band fragile, in particular against disorder effects [15, 17].

Furthermore at the c-axis oriented surface of Sr_2RuO_4, RuO_6 octahedron rotates around the c-axis with rotation angles reported as $9^\circ \pm 3^\circ$ [18] and 7.46° [16]. Our DFT calculations reveal that while this lattice distortion is irrelevant to the α and the β band structures, it leads to the change of the Fermi surface topology for the γ band, whose character changes from electron-like to hole-like one [15, 16]. The weak interlayer coupling may, therefore, yield a different Chern number close to the surface than in the bulk. The expected chiral edge current, however, never changes the flow direction around the Lifshitz transition [15], which fits well into the picture that the current is not uniquely connected with the Chern number [13, 19].

In this study we propose to examine the thermal Hall conductivity in order to detect the effect of the Lifshitz transition and the change of the topology of the chiral p-wave superconductor.

2 Model and Method

We first introduce the model Hamiltonian based on a two-dimensional tight-binding model, whose lattice structure is depicted in Fig.1. Since we focus on the connection between thermal transport properties and the topological nature, we use a single-band model resembling the γ band.

The Hamiltonian is written as

$$H = H_K + H_I, \tag{2}$$

$$H_K = -t \sum_{ij\sigma} c^\dagger_{i\sigma} c_{j\sigma} - t' \sum_{il\sigma} c^\dagger_{i\sigma} c_{l\sigma} - \mu \sum_{\sigma} n_{i\sigma}, \tag{3}$$

$$H_I = U \sum_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} + V \sum_{il\sigma\sigma'} n_{i\sigma} n_{l\sigma'}, \tag{4}$$

where $c_{i\sigma}$ ($c^\dagger_{i\sigma}$) is the annihilation (creation) operator for Ru 4d d_{xy} electrons on the site i with spin σ ($=\uparrow$ or $\downarrow$), and $n_{i\sigma}$ stands for the corresponding number operator. t and t' represent the

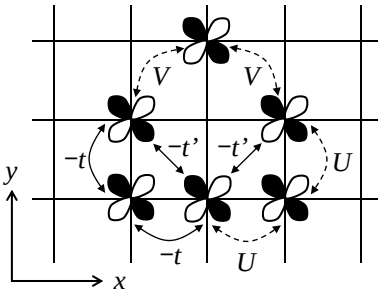

Figure 1: Lattice structure. t (t') stands for the hopping amplitude between nearest- (next-nearest-) neighbor lattice sites. U (V) represents the attractive interaction between nearest- (next-nearest-) neighbor lattice sites.

hopping amplitudes between the nearest- and next-nearest-neighbor lattice sites, respectively (Fig.1). The next-nearest-neighbor hopping amplitude are taken as $t' = 0.35t$. In order to consider the superconducting phase, we introduce attractive interactions U and V between the nearest- and next-nearest-neighbor lattice sites.

The Fermi surface of the non-interacting ($U = V = 0$) two-dimensional bulk system for several choices of the chemical potential μ is depicted in Fig. 2 where periodic boundary conditions along the x- and y-directions are taken into account. With increasing chemical potential μ, the Fermi surface switches from electron-like to hole-like character when $\mu = \mu_c$ passes through the van Hove point, i.e. a Lifshitz transition occurs at $\mu = 1.4t(\equiv \mu_c)$. The Fermi surface shapes approximately reproduce those of the γ bands obtained by DFT calculation for the several rotation angles of the RuO_6 around the c-axis. Instead of dealing with the lattice distortion and the resulting doubling of the unit cell directly, we investigate the RuO_6 rotation effect on the physical properties by tuning merely the chemical potential, where the bulk (surface) state corresponds to the present model with $\mu < \mu_c$ ($\mu > \mu_c$).

We introduce the BCS-type mean-field approximation to decouple the attractive interaction terms. The gap function for the spin-triplet sector with in-plane equal-spin pairing is defined

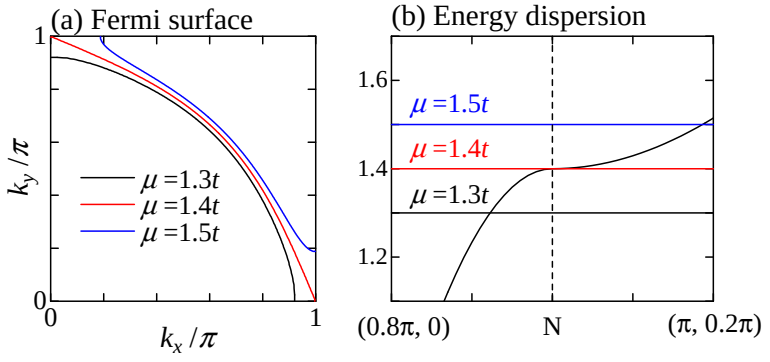

Figure 2: (Color online) (a) Fermi surface for the several choices of the chemical potential with $t' = 0.35t$ and $U = V = 0$. (b) Energy dispersion near the van Hove point and Fermi level.

as

$$\Delta_\nu = \frac{1}{2}\left\{\langle c_{i\uparrow}c_{i_\nu\downarrow}\rangle + \langle c_{i\downarrow}c_{i_\nu\uparrow}\rangle\right\}, \tag{5}$$

where i_ν stands for the nearest- ($\nu = x, y$) or next-nearest-neighbor sites ($\nu = +, -$) from i. The mean-field Hamiltonian reads

$$H^{\rm MF} = \sum_{\boldsymbol{k}} \begin{pmatrix} c^\dagger_{\boldsymbol{k}\uparrow}, & c_{-\boldsymbol{k}\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^*_{\boldsymbol{k}} & -\varepsilon_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix}, \tag{6}$$

where $c_{\boldsymbol{k}\sigma}$ ($c^\dagger_{\boldsymbol{k}\sigma}$) is the annihilation (creation) operator for Ru 4d d_{xy} electrons with wave number $\boldsymbol{k}$ and spin σ. $\varepsilon_{\boldsymbol{k}}$ and $\Delta_{\boldsymbol{k}}$ are the one-particle energy dispersion and the gap function for the spin-triplet sector, respectively, which are given by

$$\varepsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu, \tag{7}$$

$$\Delta_{\boldsymbol{k}} = 2iU\{\Delta_x \sin k_x + \Delta_y \sin k_y\} + 2iV\{\Delta_+ \sin(k_x + k_y) + \Delta_- \sin(-k_x + k_y)\}. \tag{8}$$

The order parameters are determined self-consistently for several sets of (U,V), chemical potential μ and temperature T. The most stable superconducting state is with a chiral p-wave symmetry in nearly the whole suitable parameter range, where the real and imaginary parts of the gap functions have the relative phase difference ($\pi/2$) with the same amplitudes, $\Delta_y = i\Delta_x (\equiv i\Delta)$ and $\Delta_- = i\Delta_+ (\equiv i\Delta')$ corresponding to the angular momentum of the Cooper pair $L_z = +1$. In the case of $U \neq 0$ and $V \neq 0$, the gap functions between the nearest- and next-nearest-neighbor sites have same chirality. Thus $\boldsymbol{d}$ vector is written as

$$\boldsymbol{d} = \Delta\hat{z}(\sin k_x + i \sin k_y) + \Delta'\hat{z}\{\sin(k_x + k_y) + i \sin(-k_x + k_y)\}, \tag{9}$$

where the phase difference between Δ and Δ' is $\arg(\Delta'/\Delta) = \pi/4$. Note that the minimum of the superconducting gap in the whole Brillouin zone vanishes at $\mu = \mu_c$, which is independent of the amplitudes of U and V.

3 Topological Property

In the systems with a nodeless gap, the topology of the superconducting state is characterized by the Chern number, which is defined as

$$N_c = -\frac{1}{4\pi}\int dk_x dk_y\, \hat{\boldsymbol{d}}_{\boldsymbol{k}} \cdot \left(\frac{\partial \hat{\boldsymbol{d}}_{\boldsymbol{k}}}{\partial k_x} \times \frac{\partial \hat{\boldsymbol{d}}_{\boldsymbol{k}}}{\partial k_y}\right), \tag{10}$$

$$\boldsymbol{d}_{\boldsymbol{k}} = (\mathrm{Re}\Delta_{\boldsymbol{k}}, \mathrm{Im}\Delta_{\boldsymbol{k}}, \varepsilon_{\boldsymbol{k}}),\ \hat{\boldsymbol{d}}_{\boldsymbol{k}} = \boldsymbol{d}_{\boldsymbol{k}}/|\boldsymbol{d}_{\boldsymbol{k}}|. \tag{11}$$

Figure 3 displays the Chern number as a function of the chemical potential. Even near the Lifshitz transition, the Chern number N_c never vanishes. While with $\mu < \mu_c\,(\equiv 1.4t)$ N_c is -1 and $+3$ for $(U, V) = (-2t, 0)$ and $(U, V) = (0, -2t)$ respectively, it becomes $+1$ for $\mu > \mu_c$ in both cases. Note that these amplitudes correspond to the number of edge states due to the bulk-edge correspondence.

The change of the Chern number occurs at $\mu = \mu_c$, a critical value which does not depend on the magnitude of U and V. Note that we may define the Chern number in each layer, if the layers are only weakly coupled which may be the case for the γ-band of Sr_2RuO_4, such that the bulk Chern number needs not to be identical to the one at the surface. The amplitude of the superconducting gap vanishes at the van Hove point such that at the Lifshitz transition the topological character of the γ band becomes fragile.

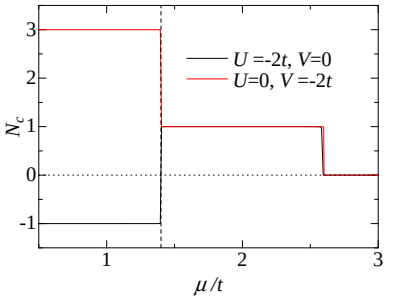

Figure 3: (Color online) The Chern number as a function of chemical potential μ for two choices of (U, V) sets at absolute zero temperature. The dashed line stands for $\mu = \mu_c$.

4 Thermal Hall Conductivity

In this section, we discuss the interplay between the topological properties and the thermal Hall effect which is the thermal analogue of the Hall effect. As a response to a thermal gradient a transverse heat flow is detected.

The thermal Hall conductivity in a chiral p-wave superconductor is given by

$$\kappa_{xy} = -\frac{1}{4\pi T}\int d\varepsilon\, \Lambda(\varepsilon) f'(\varepsilon), \tag{12}$$

$$\Lambda(\varepsilon) = \frac{4\pi}{M}\sum_{\boldsymbol{k}n} \mathrm{Im}\left\langle \frac{\partial u_{\boldsymbol{k}n}}{\partial k_x}\middle|\frac{\partial u_{\boldsymbol{k}n}}{\partial k_y}\right\rangle \theta(\varepsilon - E_{\boldsymbol{k}n}), \tag{13}$$

where T and M denote temperature and the number of lattice sites, respectively [20]. $f'(\varepsilon)$ and $\theta(\varepsilon)$ are the derivative of the Fermi-distribution function and the step function, respectively, where ε is measured relative to μ. $u_{\boldsymbol{k}n}$ is the periodic part of the Bloch wave function for wave vector $\boldsymbol{k}$ and band index n. We stress that at $\varepsilon = 0$ $\Lambda(\varepsilon)$ is an integer identical to the Chern number N_c.

The temperature dependence of the thermal Hall conductivity is depicted in Fig. 4. In the zero-temperature limit we find $\kappa_{xy} \sim (\pi N_c/12)T$ using the Sommerfeld expansion [20]. The explicit dependence on the Chern number suggests that κ_{xy} changes drastically at around the Lifshitz transition in the low-temperature limit.

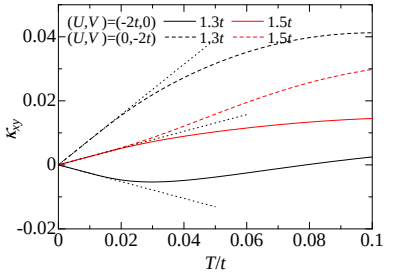

Figure 4: (Color online) The thermal Hall conductivity κ_{xy} as a function of temperature for $(U, V) = (-2t, 0)$ and $(U, V) = (0, -2t)$. The dotted lines stand for the slope of κ_{xy} at the low temperature limit.

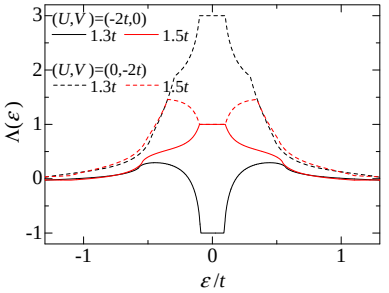

Figure 5: (Color online) $\Lambda(\varepsilon)$ for $(U,V)=(-2t,0)$ and $(U,V)=(0,-2t)$ and for $\mu=1.3t$ and $\mu=1.5t$ at absolute zero temperature.

We consider now the deviations from the T-linear behavior at very low temperatures. For this purpose it is helpful to analyze the structure of $\Lambda(\varepsilon)$ as displayed in Fig.5 for several choices of the parameters at $T=0$. In the range of $|\varepsilon|\leq\varepsilon_0$ we find $\Lambda(\varepsilon)$ to be constant N_c, where ε_0 corresponds to the (smallest) quasiparticle energy gap in the superconducting phase at zero temperature. Since the Chern number N_c jumps at the Lifshitz transition ($\mu=\mu_c$) also $\Lambda(\varepsilon)$ changes abruptly. For $|\varepsilon|>\varepsilon_0$ $\Lambda(\varepsilon)$ varies quickly and decays to zero for large $|\varepsilon|$.

Approximating the zero-temperature $\Lambda(\varepsilon)$ by a rectangular form we assume $\Lambda^R(\varepsilon)=N_c$ for $|\varepsilon|\leq\varepsilon_0$ and zero otherwise. This allows us to obtain a good account of the temperature dependence of κ_{xy} for $T\ll T_c$ where we can consider the superconducting gap essentially temperature independent. With $\Lambda^R(\varepsilon)$ we find analytically from Eq.(12),

$$\kappa_{xy}^R \approx \frac{N_c T}{2\pi}\left\{\frac{\pi^2}{6}-\gamma(T)e^{-\frac{\varepsilon_0}{T}}\right\}, \tag{14}$$

$$\gamma(T) \approx 4\left(\frac{\varepsilon_0}{2T}\right)^2+4\left(\frac{\varepsilon_0}{2T}\right)+2. \tag{15}$$

The rectangularly shaped $\Lambda^R(\varepsilon)$ not only generates the correct T-linear term but also introduces an exponential term. In order to obtain a picture of the behavior of the different parameters we replace $\gamma(T)$ by the constant β leading to the form

$$\tilde{\kappa}_{xy}=\kappa_{xy}^L+\beta e^{-\frac{\delta}{T}}. \tag{16}$$

Then we use our numerical results for Eq.(12) to fit the parameters δ and β in the low-temperature regime, where we keep $\kappa_{xy}^L(=(\pi N_c/12)T)$.

Figure 6 shows the parameters β and δ as a function of μ. Around $\mu=\mu_c$ indeed δ essentially follows ε_0 for the both sets of (U,V) considered, $(U,V)=(-2t,0)$ and $(0,-2t)$. Therefore δ vanishes together with ε_0 at $\mu=\mu_c$ where the gap has to vanish for the topological transition (Lifshitz transition).

The parameter β changes correspondingly sign at $\mu=\mu_c$. Clearly this term describes the correction to κ_{xy} due to thermal excitation of quasiparticles in the bulk beyond the gap ε_0 which disturbs the quantization. At zero-temperature κ_{xy}/T would show a sharp step. Thermal activation tends to smoothen and broaden this step. The sign of β is accordingly for the two cases of (U,V) as one can see easily. This is also reflected in the behavior of $\Lambda(\varepsilon)$ immediately beyond $|\varepsilon|=\varepsilon_0$. The rectangular approximation is well for the case $(U,V)=(-2t,0)$ for all μ, but not so for the case $(U,V)=(0,-2t)$ and $\mu>\mu_c$ as one sees comparing $\Lambda(\varepsilon)$ in Fig.5.

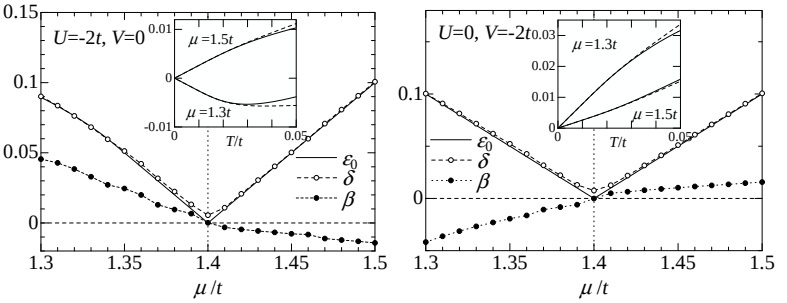

Figure 6: The fitting parameters β and δ as a function of μ for $(U, V) = (-2t, 0)$ and $(U, V) = (0, -2t)$. The insets show κ_{xy} (solid lines) and $\tilde{\kappa}_{xy}$ (dashed lines) as a function of temperature for $\mu = 1.3t$ and $\mu = 1.5t$.

5 Summary

We have investigated the connection between the thermal Hall effect and the topological property in a chiral p-wave superconductor. Using the tight-binding model describing the γ band of Sr_2RuO_4 within a self-consistent Bogoliubov-de Gennes approach, we calculate the thermal Hall conductivity and derive an analytical approximation for the low-temperature behavior. We discuss the situation of a Lifshitz transitions as a function of the chemical potential, which modifies the topological properties. Our analysis shows not only the topological quantized thermal Hall conductivity, but also the effect of thermal excitations which blur the perfect quantization. This latter feature would be important in particular at a Lifshitz transition which is simultaneously a topological transition with closing quasiparticle gap. Such a transition may be realized for the γ-band of Sr_2RuO_4 when a rotation of the RuO_6 octahedron modifying the band structure occurs. It has been suggested that this could happen at the c-axis oriented surfaces of this material.

Acknowledgments

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